	3	MI	-283.3
	4	4.4	-355.2
	5	4.2	-338.2
1gb1(8) 56 res	1	2.4	-539.6
	2	2.6	-527.7
	3	2.6	-530.2
	4	2.7	-562.3
	5	2.7	-548.0
	6	2.7	-542.0
	7	3.0	-550.5
	8	3.2	-586.7
	9	3.5	-563.7
	10	4.0	-551.0
	11	MI	-535.3
1ctf(10) 68 res	1	3.4	-710.5
	2	3.6	-758.3
	3	3.7	-720.9
	4	3.7	-746.6
	5	4.1	-622.5
	6	MI	-655.1
	7	4.6	-700.0
	8	3.8	-692.0
	9	3.2	-727.2
	10	3.8	-749.4
1pcy(46) 99 res	1	3.1	-841.8
	2	3.6	-824.5
	3	3.5	-787.2
	4	3.8	-783.3
	5	3.9	-834.7
	6	3.5	-848.0
	7	MI	-744.2
1pcy(25)	1	4.7	-944.3
	2	4.8	-786.7
	3	4.5	-898.0
	4	5.2	-928.4
1pcy(15)	1	MI	-870.7
	2	5.6	-860.8
	3	5.2	-874.7
	4	5.3	-925.1
2trx(16) 108 res	1	3.8	-1098
	2	3.5	-1089
	3	4.5	-1022
2trx(30)	1	2.8	-1036

	2	3.2	-1037
	3	3.7	-1041
	4	MI	-844
4fab(27)	1	4.5	-959
111 res	2	4.4	-1006
	3	4.9	-1037
	4	4.1	-1031
	5	MI	-984
4fab(16)	1	5.0	-1042
	2	5.1	-1062
	3	4.8	-1041
	4	5.5	-953
	5	4.9	-1035
	6	5.8	-1090
	7	MI	-1005
	8	MI	-1033
	9	MI	-1062
3fxn(35)	1	3.6	-1441
138 res	2	3.8	-1447
	3	3.6	-1432
	4	3.5	-1485
	5	4.5	-1409
	6	3.5	-1493
	7	4.4	-1464
	8	4.1	-1533
	9	MI	-1289
3fxn(20)	1	3.7	-1447
	2	3.9	-1464
	3	3.3	-1511
	4	4.2	-1515
	5	4.2	-1503
	6	4.5	-1499
1mba(20)	1	3.5	-1705
146 res	2	3.7	-1733
	3	4.1	-1705
	4	5.6	-1605
	5	4.2	-1849
	6	5.0	-1570
	7	4.1	-1741
Atim(62)	1	5.0	-2412
247 res	2	5.6	-2357
	3	5.7	-2417
	4	5.8	-2491

	5	5.4	-2499
Atim(50)	1	5.9	-2428
	2	6.5	-2507
	3	5.9	-2540
	4	6.2	-2509
Atim(36)	1	6.6	-2469
	2	6.4	-2599
	3	6.3	-2558
	4	MI	-2593
	5	6.5	-2526
	6	6.5	-2643

[a] In parentheses, the number of long-range constraints, S1, S2, . . . S5, various sets of constraints for 18-56 residue 6pti fragment.

[b] Coordinate root mean square deviation between crystallographic coordinates of Cα's and the approximate positions of the model Cα's calculated as $R^{C}_{\alpha i} = (4\mathbf{r}_i + \mathbf{r}_{i-1} + \mathbf{r}_{i+1})/6$.

[c] MI, misfolded structure that has satisfied the long-range constraints, generally the topological mirror image fold.

In the above cases, based on the conformational energy of just one (the last in a trajectory) snapshot, it was possible in all cases to identify the proper fold. However, it should be also noted that this very simple criterion may not always work. Indeed, in the case of the fourth set (S4) of long-range constraints for 6pti, the difference between the energy of a misfolded state and the lowest energy of properly folded states (simulation #3) was marginal. Moreover, the three remaining properly folded conformations have a higher energy than the misfolded one does. Fortunately, for bigger proteins, the situation is different. The energy gap between the proper fold and misfolded states is usually quite large, except for the cases where substantial all of the protein (or particular protein domain) has a β-conformation, and thus has a smallest number of long-range constraints.

The reasons for the apparently lower reliability of the β-protein prediction are complex, and several long-range constraints are required before complex β-type natural proteins can be folded. These proteins have a larger number of building blocks (compare the number of β-strands in an all-β protein with the number of helices in a helical structure of similar size) and, consequently, more complex folds.